

BUBBLES ENRICHED QUADRATIC FINITE ELEMENT METHOD FOR THE 3D-ELLIPTIC OBSTACLE PROBLEM

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ABSTRACT. Optimally convergent (with respect to the regularity) quadratic finite element method for two dimensional obstacle problem on simplicial meshes is studied in (Brezzi, Hager, Raviart, Numer. Math, 28:431–443, 1977). There was no analogue of a quadratic finite element method on tetrahedron meshes for three dimensional obstacle problem. In this article, a quadratic finite element enriched with element-wise bubble functions is proposed for the three dimensional elliptic obstacle problem. A priori error estimates are derived to show the optimal convergence of the method with respect to the regularity. Further a posteriori error estimates are derived to design an adaptive mesh refinement algorithm. Numerical experiment illustrating the theoretical result on *a priori* error estimate is presented.

1. INTRODUCTION

The obstacle problem appears in the study of elliptic variational inequalities with applications in contact mechanics, option pricing and fluid flow problems. Generally, the obstacle problem exhibits free boundary along which the regularity of the solution is influenced. The location of the free boundary is not *a priori* known and it forms a part of the numerical approximation. This makes the finite element approximation of this problem an interesting subject as it offers challenges both in the theory and the computation. we refer to the books [3, 20, 33, 40] for the theoretical and numerical aspects of variational inequalities. The finite element analysis of the obstacle problem started in 1970's, see [12, 18]. Subsequently there has been a tremendous progress on the subject, see [10, 11, 30, 42, 43] for the convergence analysis of finite element methods for the obstacle problem and see [6, 17, 27, 31] for the Signorini contact problem. The adaptive finite element methods play an important role in improving the accuracy of the numerical solution in an efficient way. A posteriori error estimates are key tools in the design of adaptive schemes, see [1] for the theory of a posteriori error analysis. In the context of the obstacle problem there has been a lot of work, see [2, 5, 8, 15, 21, 24, 34, 35, 41, 45] and see [4, 22, 23, 25, 26, 44]. Further, the convergence of adaptive methods based on a posteriori error estimates is also studied recently, see [13, 14, 19, 39, 36]. Further, we refer to [7, 28, 37, 46] for the work related to the Signorini contact problem.

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The contribution of this article is on the design and analysis of a quadratic finite element method for the three dimensional elliptic obstacle problem. The work in [12, 42] and [24] is for a quadratic finite element method (FEM) for the two dimensional obstacle problem. The quadratic FEM in two dimensions is based on the discrete constraints at the midpoints of the edges of the triangles. These constraints are shown to be enough to guarantee the convergence of the method at the rate that is optimal with respect to the regularity of the solution. The key idea in a priori error estimates in [12, 42] can be realized to be that if a quadratic function v is nonnegative at the midpoints of a triangle T , then the integral of v on T is nonnegative. This is a simple fact from the observation that the integral of a canonical P_2 -nodal basis function corresponding to a vertex on T is zero. This guides to consider the constraints at the midpoints of the edges only. However the same principle cannot be extended to three dimensional domains as the integral of a canonical P_2 -nodal basis function corresponding to a vertex is negative. The remedy we adopt in this article is by enriching the P_2 -finite element space with element-wise bubble functions and then considering the constraints on the integral mean values over each simplex in the mesh. The a priori error analysis is performed to show the convergence of the scheme. Further a posteriori error estimates are derived to design an adaptive finite element scheme. In the literature, there are hp -finite element methods available for the obstacle problem [4, 25, 26], but they use rectangular elements which are not well-suited for the adaptive mesh refinement algorithms.

Let $\Omega \subset \mathbb{R}^3$ be a bounded polyhedral domain with boundary $\partial\Omega$. Assume that the load function $f \in L^2(\Omega)$ and the obstacle $\chi \in C(\bar{\Omega}) \cap H^1(\Omega)$ satisfying $\chi|_{\partial\Omega} \leq 0$. We will also assume additional regularity on f and χ in the subsequent a priori error analysis. The admissible closed and convex set for the solution is defined by

$$\mathcal{K} = \{v \in H_0^1(\Omega) : v \geq \chi \text{ a.e. in } \Omega\}.$$

Note that since $\chi^+ = \max\{\chi, 0\} \in \mathcal{K}$, the set \mathcal{K} is nonempty. We consider the model problem of finding $u \in \mathcal{K}$ such that

$$(1.1) \quad a(u, v - u) \geq (f, v - u) \quad \text{for all } v \in \mathcal{K},$$

where for simplicity $a(u, v) = (\nabla u, \nabla v)$. Hereafter, (\cdot, \cdot) denotes the $L^2(\Omega)$ inner-product. We denote by $\|\cdot\|$ the $L^2(\Omega)$ norm. The result of Stampacchia [3, 20, 33] implies the existence of a unique solution to (1.1).

For the a posteriori error analysis, we make use of the Lagrange multiplier $\sigma \in H^{-1}(\Omega)$ defined by

$$(1.2) \quad \langle \sigma, v \rangle = (f, v) - a(u, v) \quad \text{for all } v \in H_0^1(\Omega),$$

where $\langle \cdot, \cdot \rangle$ denotes the duality bracket of $H^{-1}(\Omega)$ and $H_0^1(\Omega)$. It is useful to note from (1.2) and (1.1) that

$$(1.3) \quad \langle \sigma, v - u \rangle \leq 0 \quad \text{for all } v \in \mathcal{K}.$$

The rest of the article is organized as follows. In the Section 2, we introduce the notation, preliminaries, the discrete problem and the Lagrange multiplier for a posteriori error

estimates. In the Section 3 and 4, we derive a priori and a posteriori error estimates, respectively. In the Section 5, we propose a primal dual active set algorithm for solving the discrete problem and subsequently present a numerical experiment. Finally we conclude the article in the Section 6.

2. DISCRETE PROBLEM

2.1. Preliminaries. Let \mathcal{T}_h be a regular triangulation of Ω with simplices (tetrahedrons). A generic tetrahedron (simplex) is denoted by T and its diameter and volume by h_T and $|T|$, respectively. Set $h = \max\{h_T : T \in \mathcal{T}_h\}$. The set of all vertices of tetrahedrons that are inside Ω is denoted by \mathcal{V}_h^i . The set of all vertices that are on the boundary $\partial\Omega$ is denoted by \mathcal{V}_h^b . Set $\mathcal{V}_h = \mathcal{V}_h^i \cup \mathcal{V}_h^b$. We also use \mathcal{V}_T to denote the set of four vertices of the tetrahedron T . Let \mathcal{M}_h^i (resp. \mathcal{M}_h^b) be the set of all midpoints of the interior (resp. boundary) edges of \mathcal{T}_h and set $\mathcal{M}_h = \mathcal{M}_h^i \cup \mathcal{M}_h^b$. Further, we denote the set of midpoints of the six edges of T by \mathcal{M}_T . The set of all interior faces is denoted by \mathcal{E}_h^i . Finally, we denote the diameter of a generic face $e \in \mathcal{E}_h^i$ by h_e .

For any $e \in \mathcal{E}_h^i$, there are two simplices T_+ and T_- such that $e = \partial T_+ \cap \partial T_-$. Let n_- be the unit normal of e pointing from T_- to T_+ , and $n_+ = -n_-$. For any v which is piecewise smooth, we define the jump of ∇v on e by

$$[[\nabla v]] = \nabla v_- \cdot n_- + \nabla v_+ \cdot n_+,$$

where $v_{\pm} = v|_{T_{\pm}}$ and $v|_T$ denotes the restriction of v to T .

For any $T \in \mathcal{T}_h$ and $v \in L^1(T)$, define

$$A_T(v) = \frac{1}{|T|} \int_T v(x) dx.$$

Let $V_{pc,h} = \{v \in L^1(\Omega) : v|_T \in \mathbb{P}_0(T) \text{ for all } T \in \mathcal{T}_h\}$, where $\mathbb{P}_r(T)$ denotes the space of polynomials of total degree less than or equal to r . Define $A_h : L^1(\Omega) \rightarrow V_{pc,h}$ by $A_h(v)|_T = A_T(v)$ for all $v \in L^1(\Omega)$.

2.2. Discrete Problem. Before defining the finite element space, we define for each simplex $T \in \mathcal{T}_h$ a $P_4(T)$ bubble function b_T by

$$(2.1) \quad b_T = 256 \lambda_1^T \lambda_2^T \lambda_3^T \lambda_4^T,$$

where λ_i^T (for $i = 1, 2, 3, 4$) is the barycentric coordinate of T associated with the vertex $a_i \in \mathcal{V}_T$. Define the spaces

$$W_h = \{v_h \in H_0^1(\Omega) : v_h|_T \in \mathbb{P}_2(T) \text{ for all } T \in \mathcal{T}_h\},$$

and

$$B_h = \{v_h \in H_0^1(\Omega) : v_h|_T \in \text{span}\{b_T\} \text{ for all } T \in \mathcal{T}_h\}.$$

The finite element space V_h for approximating the obstacle problem is defined by

$$V_h = W_h \oplus B_h.$$

Define the discrete set

$$\mathcal{K}_h = \{v_h \in V_h : A_h(v_h) \geq A_h(\chi)\}.$$

The discrete problem consists of finding $u_h \in \mathcal{K}_h$ such that

$$(2.2) \quad a(u_h, v_h - u_h) \geq (f, v_h - u_h) \text{ for all } v_h \in \mathcal{K}_h.$$

In the subsequent discussion we show that the above discrete problem (2.2) has a unique solution by showing that the discrete set \mathcal{K}_h is non-empty.

Interpolation I_h : Define an interpolation operator $I_h : C(\bar{\Omega}) \rightarrow V_h$ by the following: Let $v \in C(\bar{\Omega})$ and define $I_h v$ by its nodal values

$$(2.3) \quad I_h v(p) = v(p) \quad \forall p \in \mathcal{V}_h \cup \mathcal{M}_h,$$

$$(2.4) \quad A_T(I_h v) = A_T(v) \quad \forall T \in \mathcal{T}_h.$$

Define I_T by $I_T v = (I_h v)|_T$ for $v \in C(\bar{\Omega})$. The interpolation operator I_h is well-defined and satisfies $I_T v = v$ for any $v \in \mathbb{P}_2(T)$. Therefore the following approximation properties hold by the Bramble-Hilbert Lemma and scaling [9, 16]:

Lemma 2.1. *Let $v \in H^s(T)$ for $2 \leq s \leq 3$ and $T \in \mathcal{T}_h$. Then*

$$\begin{aligned} |v - I_T v|_{H^m(T)} &\leq Ch_T^{s-m} |v|_{H^s(T)}, \text{ for } 0 \leq m \leq s, \\ \|v - A_T(v)\|_{L^2(T)} &\leq Ch_T^r |v|_{H^r(T)}, \end{aligned}$$

where $0 \leq r \leq 1$.

We remark here that in the subsequent *a priori* error analysis, the interpolation I_h gives good control for the terms near the free boundary, see for example (3.4), apart from preserving the integral sign.

Since $u \geq \chi$, it is clear that $I_h u \in \mathcal{K}_h$ and hence the set \mathcal{K}_h is nonempty. Now as in the case of continuous problem (1.1), the discrete problem (2.2) can be shown to have a unique solution. The *a posteriori* error analysis will make use of a discrete Lagrange multiplier σ_h analogous to σ in (1.2). Before defining it, we note the following facts about the discrete solution u_h :

Let $z_h \in V_h$ with $A_h(z_h) \geq 0$. Then, we have $u_h + z_h \in \mathcal{K}_h$. By taking $v_h = u_h + z_h$ in (2.2), we find

$$(2.5) \quad a(u_h, z_h) \geq (f, z_h).$$

Let $v_h \in V_h$ with $A_h(v_h) = 0$. Then, by taking $z_h = \pm v_h$ in (2.5), we find

$$(2.6) \quad a(u_h, v_h) = (f, v_h).$$

Suppose for any $T \in \mathcal{T}_h$, $A_T(u_h) > A_T(\chi)$. Then by taking $v_h^\pm = u_h \pm \delta b_T$ for some sufficiently small $\delta > 0$, we find

$$a(u_h, b_T) = (f, b_T),$$

where b_T is the bubble function defined in (2.1) on T and extended by zero on $\bar{\Omega} \setminus T$. Therefore

$$(2.7) \quad a(u_h, b_T) = (f, b_T) \quad \text{for all } T \in \{T' \in \mathcal{T}_h : A_{T'}(u_h) > A_{T'}(\chi)\}.$$

Lemma 2.2. *The map $\Pi_h : V_h \rightarrow V_{pc,h}$ defined by $\Pi_h(v_h) = A_h(v_h)$ is onto and hence an inverse map $\Pi_h^{-1} : V_{pc,h} \rightarrow V_h$ can be defined into a subset of V_h such that $\Pi_h^{-1}(w_h) = v_h$ where $v_h \in V_h$ with $A_h(v_h) = w_h$ for $w_h \in V_{pc,h}$.*

Proof. For given any $w_h \in V_{pc,h}$, we prove that there is some $v_h \in V_h$ such that $A_h(v_h) = w_h$. Note that, we can write $v_h \in V_h$ as $v_h = v_1 + v_2$, where $v_1 \in W_h$ and $v_2 \in B_h$. We choose first some $v_1 \in W_h$, and then we choose $v_2 \in B_h$ such that $A_h(v_2) = w_h - A_h(v_1)$. In particular, we can choose v_1 to be zero and v_2 to be such that $v_2 \in B_h$ with $v_2|_T = w_h b_T / A_h(b_T)$. This proves that Π_h is onto. Define Π_h^{-1} by $\Pi_h^{-1}(w_h) = v_h$ where $v_h \in V_h$ is such that $A_h(v_h) = w_h$ for $w_h \in V_{pc,h}$. Again v_h can be chosen such that $v_h|_T = w_h b_T / A_h(b_T)$. \square

Define the discrete Lagrange multiplier $\sigma_h \in V_{pc,h}$ by

$$(2.8) \quad (\sigma_h, w_h) = (f, \Pi_h^{-1} w_h) - a(u_h, \Pi_h^{-1} w_h) \quad \forall w_h \in V_{pc,h},$$

where Π_h^{-1} is defined as in Lemma 2.2.

The following lemma proves some properties of σ_h .

Lemma 2.3. *The discrete Lagrange multiplier defined by (2.8) is well-defined. Further*

$$(2.9) \quad \sigma_h \leq 0 \quad \text{on } \bar{\Omega},$$

and

$$(2.10) \quad \sigma_h|_T = 0 \quad \text{for all } T \in \{T' \in \mathcal{T}_h : A_{T'}(u_h) > A_{T'}(\chi)\}.$$

Proof. For $w_h \in V_{pc,h}$, let v_1 and $v_2 \in V_h$ be such that $v_1 \neq v_2$ and $\Pi_h(v_1) = \Pi_h(v_2) = w_h$, where Π_h is defined as in Lemma 2.2. Then since $A_h(v_1 - v_2) = 0$, we have by (2.6) that $a(u_h, v_1 - v_2) = (f, v_1 - v_2)$. This implies $a(u_h, v_1) - (f, v_1) = a(u_h, v_2) - (f, v_2)$ and hence σ_h is well-defined.

Choosing $w_h \geq 0$ in (2.8) and using (2.5) we conclude that $\sigma_h \leq 0$ on $\bar{\Omega}$. Similarly (2.10) follows from (2.7). \square

In view of the Lemma 2.3 and since we can chose $\Pi_h^{-1}(w_h)$ element-wise by $\Pi_h^{-1}(w_h)|_T = w_h b_T / A_h(b_T)$, it is easy to see that we can write (2.8) element-wise as

$$(2.11) \quad \sigma_h|_T = \left(\int_T b_T dx \right)^{-1} \left(\int_T f b_T dx - \int_T \nabla u_h \cdot \nabla b_T dx \right).$$

The above formula is useful in computing the σ_h . Further, for any $v_h \in V_h$ we have by (2.8) that

$$(\sigma_h, A_h(v_h)) = (f, v_h) - a(u_h, v_h) \quad \forall v_h \in V_h.$$

But since $(\sigma_h, v_h) = (\sigma_h, A_h(v_h))$, we finally have

$$(2.12) \quad (\sigma_h, v_h) = (f, v_h) - a(u_h, v_h) \quad \forall v_h \in V_h.$$

3. A PRIORI ERROR ANALYSIS

The regularity theory of obstacle problem [33, Theorem 2.5] implies that if $f \in L^2(\Omega)$, $\chi \in H^2(\Omega)$ and Ω is convex, then the solution $u \in H^2(\Omega)$. In particular the Lagrange multiplier σ defined in (1.2) can be written as $\sigma = f + \Delta u$ and hence $\sigma \in L^2(\Omega)$. The following lemma follows from (1.1) and (1.2), see [33, 20]:

Lemma 3.1. *If $u \in H^2(\Omega)$, then $\sigma \in L^2(\Omega)$ and*

$$\begin{aligned} \sigma &\leq 0 \quad \text{a.e. in } \Omega, \\ (\sigma, u - \chi) &= 0. \end{aligned}$$

Further if $u > \chi$ on some open set $D \subset \Omega$, then $\sigma \equiv 0$ on D .

For the rest of this section, we assume that the data $f \in H^1(\Omega)$, $\chi \in H^3(\Omega)$ and the solution $u \in H^3(\Omega_N) \cup H^3(\Omega_C)$, where

$$\begin{aligned} \Omega_N &= \{x \in \Omega : u(x) > \chi(x)\}, \\ \Omega_C &= \{x \in \Omega : u(x) = \chi(x)\}^\circ, \end{aligned}$$

for any set $D \subset \Omega$, the set D° denotes the interior of D . Further assume that $u \in H^s(\Omega)$, where $s = 5/2 - \epsilon$ for any $\epsilon > 0$. We derive now an a priori error estimate. This regularity assumption makes sense as the solution of the obstacle problem loses the regularity at the free boundary and if the free boundary is smooth the solution satisfies as elliptic problem in the non contact region. Further, on the contact region, the obstacle is assumed to be smooth enough.

Theorem 3.2. *There holds*

$$\|\nabla(u - u_h)\| \leq Ch^{3/2-\epsilon} (\|u\|_{H^{5/2-\epsilon}(\Omega)} + \|f\|_{H^1(\Omega)} + \|\chi\|_{H^3(\Omega)} + \|u\|_{H^3(\Omega_N)}),$$

for any $\epsilon > 0$.

Proof. Since $I_h u \in \mathcal{K}_h$, we find using (2.2) and integration by parts that

$$\begin{aligned} \|\nabla(u - u_h)\|^2 &= a(u - u_h, u - I_h u) + a(u - u_h, I_h u - u_h) \\ &\leq a(u - u_h, u - I_h u) + a(u, I_h u - u_h) - (f, I_h u - u_h) \\ &= a(u - u_h, u - I_h u) + (-\Delta u - f, I_h u - u_h) \\ &= a(u - u_h, u - I_h u) - \sum_{T \in \mathcal{T}_h} \int_T \sigma(I_h u - u_h) dx. \end{aligned}$$

The interpolation properties of I_h in Lemma 2.1 imply that

$$(3.1) \quad \|\nabla(u - I_h u)\| \leq Ch^{3/2-\epsilon} \|u\|_{H^{5/2-\epsilon}(\Omega)},$$

for any $\epsilon > 0$. On the other hand, divide the elements in \mathcal{T}_h into the following sets:

$$\begin{aligned} \mathbb{N} &= \{T \in \mathcal{T}_h : u > \chi \text{ on } T\}, \\ \mathbb{C} &= \{T \in \mathcal{T}_h : u \equiv \chi \text{ on } T\}, \end{aligned}$$

$$\mathbb{F} = \mathcal{T}_h \setminus \{\mathbb{N} \cup \mathbb{C}\}.$$

Then we write

$$\begin{aligned}
 \sum_{T \in \mathcal{T}_h} \int_T \sigma(I_h u - u_h) dx &= \sum_{T \in \mathbb{N}} \int_T \sigma(I_h u - u_h) dx + \sum_{T \in \mathbb{C}} \int_T \sigma(I_h u - u_h) dx \\
 &\quad + \sum_{T \in \mathbb{F}} \int_T \sigma(I_h u - u_h) dx \\
 (3.2) \qquad &= \sum_{T \in \mathbb{C}} \int_T \sigma(I_h u - u_h) dx + \sum_{T \in \mathbb{F}} \int_T \sigma(I_h u - u_h) dx,
 \end{aligned}$$

since on any $T \in \mathbb{N}$, we have $\sigma \equiv 0$ on T . Also since $A_T(\sigma) \leq 0$ for any $T \in \mathcal{T}_h$, we have

$$\int_T A_T(\sigma)(I_h \chi - u_h) dx \geq 0 \quad \forall T \in \mathcal{T}_h.$$

Now let $T \in \mathbb{C}$. Then we have $u \equiv \chi$ on T and

$$\begin{aligned}
 \int_T \sigma(I_h u - u_h) dx &= \int_T \sigma(I_h \chi - u_h) dx \geq \int_T (\sigma - A_T(\sigma))(I_h \chi - u_h) dx \\
 &= \int_T (\sigma - A_T(\sigma))(I_h u - u_h) dx \\
 &= \int_T (\sigma - A_T(\sigma))((I_h u - u_h) - A_T(I_h u - u_h)) dx \\
 (3.3) \qquad &\geq -Ch_T^2 \|\sigma\|_{H^1(T)} \|\nabla(I_h u - u_h)\|_{L^2(T)}.
 \end{aligned}$$

Finally let $T \in \mathbb{F}$. Then using Lemma 3.1, we find

$$\begin{aligned}
 \int_T \sigma(I_h u - u_h) dx &= \int_T \sigma((I_h u - u) + (u - \chi) + (\chi - I_h \chi) + (I_h \chi - u_h)) dx \\
 &= \int_T \sigma(I_h(u - \chi) - (u - \chi) + (I_h \chi - u_h)) dx.
 \end{aligned}$$

Using the definition and interpolation properties of I_h , we find

$$\begin{aligned}
 \left| \int_T \sigma(I_h(u - \chi) - (u - \chi)) dx \right| &= \left| \int_T (\sigma - A_T(\sigma))(I_h(u - \chi) - (u - \chi)) dx \right| \\
 &\leq Ch_T^{1/2-\epsilon} \|(u - \chi) - I_h(u - \chi)\|_{L^2(T)} \|\sigma\|_{H^{1/2-\epsilon}(T)} \\
 (3.4) \qquad &\leq Ch_T^{3-2\epsilon} \|u - \chi\|_{H^{5/2-\epsilon}(T)} \|\sigma\|_{H^{1/2-\epsilon}(T)},
 \end{aligned}$$

for any $\epsilon > 0$. As for $T \in \mathbb{C}$, we note for any $\epsilon > 0$ that

$$\begin{aligned}
 \int_T \sigma(I_h \chi - u_h) dx &\geq \int_T (\sigma - A_T(\sigma))(I_h \chi - u_h) dx \\
 &= \int_T (\sigma - A_T(\sigma))((I_h \chi - u_h) - A_T(I_h \chi - u_h)) dx
 \end{aligned}$$

$$\geq -Ch_T^{3/2-\epsilon} \|\sigma\|_{H^{1/2-\epsilon}(T)} \|\nabla(I_h\chi - u_h)\|_{L^2(T)}.$$

Using the triangle inequality and interpolation properties of I_h , we find

$$\begin{aligned} \|\nabla(I_h\chi - u_h)\|_{L^2(T)} &\leq \|\nabla(I_h\chi - \chi)\|_{L^2(T)} + \|\nabla(\chi - u)\|_{L^2(T)} + \|\nabla(u - u_h)\|_{L^2(T)} \\ &\leq Ch_T^2 \|\chi\|_{H^3(T)} + \|\nabla(u - \chi)\|_{L^2(T)} + \|\nabla(u - u_h)\|_{L^2(T)}. \end{aligned}$$

Note that if $u - \chi = 0$ on a set D of measure non zero, then by the result of Stampachchia, $\nabla(u - \chi) = 0$ a.e. on D , see [32, Appendix 4]. Therefore

$$\|\nabla(u - \chi)\|_{L^2(T)} = \left(\int_{\{u > \chi\}} |\nabla(u - \chi)|^2 dx \right)^{1/2} = \|\nabla(u - \chi)\|_{L^2(E)},$$

where $E = \{x \in T : u(x) - \chi(x) > 0\}$. Since $u - \chi \in C(\bar{\Omega})$, the set E is open. From the assumption on the regularity, we have $u - \chi \in H^3(E)$. Since $H^3(E) \subset C^{1,\theta}(\bar{E})$ with $\theta = 1/2$, we have from [32, Theorem 2.4.5] that

$$|\nabla(u - \chi)(x)| \leq C|x - x^*|^{1/2} \|u - \chi\|_{H^3(E)},$$

where $x \in E$ and $x^* \in \partial E$ is such that $\nabla(u - \chi)(x^*) = 0$. Therefore

$$\|\nabla(u - \chi)\|_{L^2(T)} \leq C|T|^{1/2} h_T^{1/2} \|u - \chi\|_{H^3(E)} \leq Ch_T^2 \|u - \chi\|_{H^3(E)}.$$

Therefore for any $T \in \mathbb{F}$, we find

$$\begin{aligned} \int_T \sigma(I_h u - u_h) dx &\geq -Ch_T^{3-2\epsilon} \|u - \chi\|_{H^{5/2-\epsilon}(T)} \|\sigma\|_{H^{1/2-\epsilon}(T)} \\ &\quad - Ch_T^{3/2-\epsilon} \|\sigma\|_{H^{1/2-\epsilon}(T)} (h_T^2 \|\chi\|_{H^3(T)} + h_T^2 \|u - \chi\|_{H^3(E)}) \\ &\quad - Ch_T^{3/2-\epsilon} \|\sigma\|_{H^{1/2-\epsilon}(T)} \|\nabla(u - u_h)\|_{L^2(T)}, \end{aligned} \tag{3.5}$$

where $E = \{x \in T : u(x) - \chi(x) > 0\}$. We complete the proof by combining the estimates in (3.1)-(3.5) \square

A priori error estimates for σ_h . In this section, we show that the discrete function σ_h converges to σ in the H^{-1} norm at the same order of convergence as that of the error $u - u_h$ in the H^1 norm. This is essential as the local efficiency estimates are derived using the combined norm of the error $u - u_h$ and the dual norm of $\sigma - \sigma_h$.

Let $(\cdot, \cdot)_T$ denote the $L^2(T)$ -inner product. Then from (1.2) and (2.8), we note that

$$(\sigma - \sigma_h, b_T)_T = (\nabla(u_h - u), \nabla b_T)_T. \tag{3.6}$$

We prove the estimate in H^{-1} norm. Let $D \subset \Omega$ be an open set and for $v \in H^{-1}(D)$ define its $H^{-1}(D)$ norm by

$$\|v\|_{H^{-1}(D)} = \sup_{\phi \in H_0^1(D), \phi \neq 0} \frac{\langle v, \phi \rangle}{\|\nabla \phi\|_{L^2(D)}}.$$

Theorem 3.3. *Let σ and σ_h be defined by (1.2) and (2.8). Then, there holds*

$$\|\sigma - \sigma_h\|_{H^{-1}(T)} \leq C \left(h_T \|\sigma - A_T(\sigma)\|_{L^2(T)} + \|\nabla(u - u_h)\|_{L^2(T)} \right).$$

Proof. Using the triangle inequality, we write

$$\begin{aligned} \|\sigma - \sigma_h\|_{H^{-1}(T)} &= \|\sigma - A_T(\sigma)\|_{H^{-1}(T)} + \|A_T(\sigma) - \sigma_h\|_{H^{-1}(T)} \\ &\leq C \left(h_T \|\sigma - A_T(\sigma)\|_{L^2(T)} + \|A_T(\sigma) - \sigma_h\|_{H^{-1}(T)} \right). \end{aligned}$$

Let $\phi \in H_0^1(T)$ and $\phi_T = (1, \phi)_T$. Then

$$(A_T(\sigma) - \sigma_h, \phi)_T = (A_T(\sigma) - \sigma_h, \phi)_T = \phi_T(1, b_T)_T^{-1} (A_T(\sigma) - \sigma_h, b_T)_T.$$

Note that by scaling $|\phi_T| \leq Ch_T^{3/2} \|\phi\|_{L^2(T)} \leq Ch_T^{5/2} \|\nabla\phi\|_{L^2(T)}$ and $(1, b_T)_T^{-1} \leq Ch_T^{-3}$. Therefore

$$|\phi_T(1, b_T)_T^{-1}| \leq Ch_T^{-1/2} \|\nabla\phi\|_{L^2(T)}.$$

Further $\|b_T\|_{L^2(T)} \leq Ch_T^{3/2}$ and $\|\nabla b_T\|_{L^2(T)} \leq Ch_T^{1/2}$. Using this we find

$$\begin{aligned} (A_T(\sigma) - \sigma_h, b_T)_T &= (A_T(\sigma) - \sigma, b_T)_T + (\sigma - \sigma_h, b_T)_T \\ &= (A_T(\sigma) - \sigma, b_T)_T + a(u_h - u, b_T)_T \\ &\leq Ch_T^{3/2} \|A_T(\sigma) - \sigma\|_{L^2(T)} + Ch_T^{1/2} \|\nabla(u - u_h)\|_{L^2(T)}, \end{aligned}$$

and

$$|\phi_T(1, b_T)_T^{-1} (A_T(\sigma) - \sigma_h, b_T)_T| \leq C \left(h_T \|A_T(\sigma) - \sigma\|_{L^2(T)} + \|\nabla(u - u_h)\|_{L^2(T)} \right) \|\nabla\phi\|_{L^2(T)},$$

which proves

$$\|A_T(\sigma) - \sigma_h\|_{H^{-1}(T)} \leq C \left(h_T \|A_T(\sigma) - \sigma\|_{L^2(T)} + \|\nabla(u - u_h)\|_{L^2(T)} \right).$$

This completes the proof. \square

Theorem 3.4. *Let σ and σ_h be defined by (1.2) and (2.8). Then, there holds*

$$\|\sigma - \sigma_h\|_{L^2(T)} \leq C \left(\|A_T(\sigma) - \sigma\|_{L^2(T)} + h_T^{-1} \|\nabla(u - u_h)\|_{L^2(T)} \right).$$

Proof. Using the triangle inequality, we find

$$\|\sigma - \sigma_h\|_{L^2(T)} = \|\sigma - A_T(\sigma)\|_{L^2(T)} + \|A_T(\sigma) - \sigma_h\|_{L^2(T)}.$$

Since $w_T = A_T(\sigma) - \sigma_h|_T \in \mathbb{P}_0(T)$, $|(1, b_T)_T| \approx Ch_T^3$ and by the scaling arguments, we find for some positive constant C that

$$\begin{aligned} C \|A_T(\sigma) - \sigma_h\|_{L^2(T)}^2 &\leq (A_T(\sigma) - \sigma_h, w_T b_T) = (A_T(\sigma) - \sigma, w_T b_T) + (\sigma - \sigma_h, w_T b_T) \\ &\leq \|\sigma - A_T(\sigma)\|_{L^2(T)} \|w_T\|_{L^2(T)} + |w_T| a(u_h - u, b_T) \\ &\leq \|\sigma - A_T(\sigma)\|_{L^2(T)} \|w_T\|_{L^2(T)} + Ch_T^{-1} \|\nabla(u - u_h)\|_{L^2(T)} \|w_T\|_{L^2(T)}. \end{aligned}$$

This completes the proof. \square

4. A POSTERIORI ERROR ESTIMATES

In this section, we derive residual based a posteriori error estimates. Note that we assume $f \in L^2(\Omega)$ and $\chi \in H^1(\Omega) \cap C(\bar{\Omega})$ and $\chi|_{\partial\Omega} \leq 0$ as in the introduction. We begin by defining the following sets:

$$\mathbb{C}_h = \{T \in \mathcal{T}_h : A_T(u_h) = A_T(\chi)\},$$

and

$$\mathbb{N}_h = \{T \in \mathcal{T}_h : A_T(u_h) > A_T(\chi)\}.$$

The residual based error estimates can be derived conveniently by using the corresponding residual. Define the residual $\mathcal{R}_h : H_0^1(\Omega) \rightarrow \mathbb{R}$ by

$$(4.1) \quad \mathcal{R}_h(v) = a(u - u_h, v) + \langle \sigma - \sigma_h, v \rangle \quad \forall v \in H_0^1(\Omega).$$

The following lemma connects the norm of the residual and the norms of the errors:

Lemma 4.1. *There holds*

$$\|\nabla(u - u_h)\|^2 + \|\sigma - \sigma_h\|_{H^{-1}(\Omega)}^2 \leq 5\|\mathcal{R}_h\|_{H^{-1}(\Omega)}^2 - 6\langle \sigma - \sigma_h, u - u_h \rangle.$$

Proof. Using (4.1) and Young's inequality, we find

$$\begin{aligned} \|\nabla(u - u_h)\|^2 &= a(u - u_h, u - u_h) = \mathcal{R}_h(u - u_h) - \langle \sigma - \sigma_h, u - u_h \rangle \\ &\leq \|\mathcal{R}_h\|_{H^{-1}(\Omega)} \|\nabla(u - u_h)\| - \langle \sigma - \sigma_h, u - u_h \rangle \\ &\leq \frac{1}{2}\|\mathcal{R}_h\|_{H^{-1}(\Omega)}^2 + \frac{1}{2}\|\nabla(u - u_h)\|^2 - \langle \sigma - \sigma_h, u - u_h \rangle, \end{aligned}$$

and

$$(4.2) \quad \|\nabla(u - u_h)\|^2 \leq \|\mathcal{R}_h\|_{H^{-1}(\Omega)}^2 - 2\langle \sigma - \sigma_h, u - u_h \rangle.$$

Using again (4.1), we note that

$$\|\sigma - \sigma_h\|_{H^{-1}(\Omega)} \leq \|\mathcal{R}_h\|_{H^{-1}(\Omega)} + \|\nabla(u - u_h)\|.$$

Now Young's inequality and (4.2) imply

$$(4.3) \quad \begin{aligned} \|\sigma - \sigma_h\|_{H^{-1}(\Omega)}^2 &\leq 2\|\mathcal{R}_h\|_{H^{-1}(\Omega)}^2 + 2\|\nabla(u - u_h)\|^2 \\ &\leq 4\|\mathcal{R}_h\|_{H^{-1}(\Omega)}^2 - 4\langle \sigma - \sigma_h, u - u_h \rangle. \end{aligned}$$

The proof then follows by combining the estimates in (4.2)-(4.3). \square

Define the following estimators:

$$\eta_1 = \left(\sum_{T \in \mathcal{T}_h} h_T^2 \|\Delta u_h + f - \sigma_h\|_{L^2(T)}^2 \right)^{1/2},$$

and

$$\eta_2 = \left(\sum_{e \in \mathcal{E}_h^i} h_e \|\llbracket \nabla u_h \rrbracket\|_{L^2(e)}^2 \right)^{1/2}.$$

The norm of the residual \mathcal{R}_h is estimated by using the error estimators in the following lemma:

Lemma 4.2. *It holds that*

$$\|\mathcal{R}_h\|_{H^{-1}(\Omega)} \leq C (\eta_1^2 + \eta_2^2)^{1/2}.$$

Proof. Let $v \in H_0^1(\Omega)$ and choose $v_h \in V_h$ be such that there holds the following approximation properties:

$$h_T^{-1} \|v - v_h\|_{L^2(T)} + \|\nabla v_h\|_{L^2(T)} \leq C \|\nabla v\|_{L^2(\mathcal{T}_T)},$$

where \mathcal{T}_T is the union of triangles contained in patches of all three vertices of T . For example, v_h can taken to be a Scott-Zhang interpolation [38]. Then

$$(4.4) \quad \langle \mathcal{R}_h, v \rangle = \langle \mathcal{R}_h, v - v_h \rangle + \langle \mathcal{R}_h, v_h \rangle.$$

Firstly using (4.1), (1.2) and (2.12), we find

$$\begin{aligned} \langle \mathcal{R}_h, v_h \rangle &= a(u - u_h, v_h) + \langle \sigma - \sigma_h, v_h \rangle \\ &= (f, v_h) - a(u_h, v_h) - (\sigma_h, v_h) = 0. \end{aligned}$$

Secondly using (4.1) and integration by parts, we find

$$\begin{aligned} \langle \mathcal{R}_h, v - v_h \rangle &= a(u - u_h, v - v_h) + \langle \sigma - \sigma_h, v - v_h \rangle \\ &= (f, v - v_h) - a(u_h, v - v_h) - (\sigma_h, v - v_h) \\ &= \sum_{T \in \mathcal{T}_h} \int_T (f + \Delta u_h - \sigma_h)(v - v_h) dx - \sum_{T \in \mathcal{T}_h} \int_{\partial T} \frac{\partial u_h|_T}{\partial n_T} (v - v_h) ds \\ &= \sum_{T \in \mathcal{T}_h} \int_T (f + \Delta u_h - \sigma_h)(v - v_h) dx - \sum_{e \in \mathcal{E}_h^i} \int_e \llbracket \nabla u_h \rrbracket (v - v_h) ds \\ &\leq C (\eta_1^2 + \eta_2^2)^{1/2} \|\nabla v\|. \end{aligned}$$

This completes the proof. \square

It remains to find a lower bound for $\langle \sigma - \sigma_h, u - u_h \rangle$. To this end, let $v^+ = \max\{v, 0\}$ and $v^- = \max\{-v, 0\}$ for any $v \in H^1(\Omega)$. Then $v = v^+ - v^-$.

Lemma 4.3. *There holds*

$$\langle \sigma - \sigma_h, u - u_h \rangle \geq -\frac{1}{12} \|\sigma - \sigma_h\|_{H^{-1}(\Omega)}^2 - C (\|\nabla(\chi - u_h)^+\|^2) + \sum_{T \in \mathcal{C}_h} \int_T \sigma_h (\chi - u_h)^- dx.$$

Proof. Let $u_h^* = \max\{u_h, \chi\}$. Then $u_h^* \in \mathcal{K}$ and $u_h^* - u_h = (\chi - u_h)^+$. Using (1.3) and $ab \leq 3a^2 + b^2/12$, we find

$$\begin{aligned} \langle \sigma, u - u_h \rangle &= \langle \sigma, u - u_h^* \rangle + \langle \sigma, u_h^* - u_h \rangle \geq \langle \sigma, u_h^* - u_h \rangle \\ &= \langle \sigma - \sigma_h, u_h^* - u_h \rangle + \langle \sigma_h, u_h^* - u_h \rangle \\ &\geq -\frac{1}{12} \|\sigma - \sigma_h\|_{H^{-1}(\Omega)}^2 - 3 \|\nabla(u_h^* - u_h)\|^2 + \langle \sigma_h, u_h^* - u_h \rangle. \end{aligned}$$

Therefore

$$\langle \sigma - \sigma_h, u - u_h \rangle \geq -\frac{1}{12} \|\sigma - \sigma_h\|_{H^{-1}(\Omega)}^2 - 3 \|\nabla(\chi - u_h)^+\|^2 + \langle \sigma_h, (u_h^* - u_h) - (u - u_h) \rangle.$$

Using the fact that $\chi - u \leq 0$ a.e. in Ω and $\sigma_h \leq 0$ on $\bar{\Omega}$, we find

$$\langle \sigma_h, (u_h^* - u_h) - (u - u_h) \rangle \geq \langle \sigma_h, (u_h^* - u_h) - (\chi - u_h) \rangle.$$

Note that as $(u_h^* - u_h) - (\chi - u_h) = (\chi - u_h)^-$, we have

$$\langle \sigma_h, (u_h^* - u_h) - (u - u_h) \rangle \geq \langle \sigma_h, (\chi - u_h)^- \rangle = \int_{\Omega} \sigma_h (\chi - u_h)^- dx.$$

Now using Lemma 2.3,

$$\int_{\Omega} \sigma_h (\chi - u_h)^- dx = \sum_{T \in \mathbb{C}_h} \int_T \sigma_h (\chi - u_h)^- dx.$$

This completes the proof. \square

From Lemma 4.1, Lemma 4.2 and Lemma 4.3, we deduce the following result on *a posteriori* error control of quadratic FEM:

Theorem 4.4. *It holds that*

$$\|\nabla(u - u_h)\|^2 + \|\sigma - \sigma_h\|_{H^{-1}(\Omega)}^2 \leq C \left(\eta_1^2 + \eta_2^2 + \|\nabla(\chi - u_h)^+\|^2 - \sum_{T \in \mathbb{C}_h} \int_T \sigma_h (\chi - u_h)^- dx \right).$$

The following local efficiency estimates can be proved easily using the bubble function techniques and the definition of σ in (1.2):

Lemma 4.5. *There hold*

$$\begin{aligned} h_T \|f + \Delta u_h - \sigma_h\|_{L^2(T)} &\leq C \left(\|\nabla(u - u_h)\|_{L^2(T)} + \|\sigma - \sigma_h\|_{H^{-1}(T)} + h_T \inf_{\bar{f} \in \mathbb{P}_0(T)} \|f - \bar{f}\|_{L^2(T)} \right) \\ h_e^{1/2} \|[\nabla u_h]\|_{L^2(e)} &\leq C \left(\|\nabla(u - u_h)\|_{L^2(T_e)} + \|\sigma - \sigma_h\|_{H^{-1}(T_e)} + h_e \inf_{\bar{f} \in \mathbb{P}_0(T_e)} \|f - \bar{f}\|_{L^2(T_e)} \right), \end{aligned}$$

where T_e is the patch of the face $e \in \mathcal{E}_h^i$.

Remark 4.6. In view of Braess [8], the terms

$$\|\nabla(\chi - u_h)^+\| \quad \text{and} \quad - \sum_{T \in \mathbb{C}_h} \int_T \sigma_h(\chi - u_h)^- dx$$

are of higher order.

5. NUMERICAL IMPLEMENTATION

In this section, first we discuss the primal-dual active set method and then present numerical experiment.

5.1. Implementation procedure. We propose the primal-dual active set method for the numerical experiments. In the light of the algorithm in [29], we develop the following algorithm for solving the 3D-obstacle problem by the quadratic finite element method developed in this article. For the given mesh size h , let \mathcal{T}_h be the simplicial triangulation of $\Omega \subset \mathbb{R}^3$ with number of simplices denoted by M . Let the simplices be enumerated by $\{T_j\}_{1 \leq j \leq M}$. Let N be the dimension of V_h and $\{\phi_i\}_{1 \leq i \leq N}$ be its basis. Denote by $A = [A_{ij}]_{1 \leq i, j \leq N}$ the stiffness matrix, where

$$A_{ij} = (\nabla \phi_j, \nabla \phi_i).$$

Define the matrix $B = [B_{ij}]_{1 \leq i \leq M, 1 \leq j \leq N}$ where

$$B_{ij} = \frac{1}{|T_j|} \int_{T_j} \phi_i dx.$$

The load vector $b = [b_i]_{1 \leq i \leq N}$ is defined as

$$b_i = (f, \phi_i).$$

Also define $\gamma = [\gamma_j]_{1 \leq j \leq M}$, where

$$\gamma_j = \frac{1}{|T_j|} \int_{T_j} \chi dx.$$

Let the discrete solution $u_h \in V_h$ be represented by

$$u_h = \sum_{i=1}^N \alpha_i \phi_i.$$

The Lagrange multiplier $\sigma_h \in V_{pc,h}$ which will be written as

$$\sigma_h = \sum_{j=1}^M \beta_j \psi_j,$$

where ψ_j is the characteristic function of T_j defined by

$$A\alpha + B\beta = b,$$

with $\alpha = [\alpha_i]_{\{1 \leq i \leq N\}}$ and $\beta = [\beta_j]_{\{1 \leq j \leq M\}}$. The complementarity conditions are given by

$$(5.1) \quad \beta^T (B^T \alpha - \gamma) = 0, \quad \beta \leq 0, \quad \text{and} \quad B^T \alpha - \gamma \geq 0.$$

The complementarity conditions can be written as

$$C(\alpha, \beta) = 0,$$

where

$$C(\alpha, \beta) = \beta - \min\{0, \beta + c(B^T \alpha - \gamma)\},$$

for some $c > 0$. Finally let $\Lambda = \{1, 2, \dots, M\}$ be the index set of mesh elements $T_j \in \mathcal{T}_h$.

The primal-dual active set algorithm is defined as follows:

Algorithm 5.1. Initialize α^0 and β^0 . Let $k = 1$, $\alpha^1 = \alpha^0$ and $\beta^1 = \beta^0$. For $k \geq 1$, perform the following steps:

Step 1. Find $A_k = \{j \in \Lambda : \beta_j^k + c(B^T \alpha^k - \gamma)_j < 0\}$ and $I_k = \{j \in \Lambda : \beta_j^k + c(B^T \alpha^k - \gamma)_j \geq 0\}$.

Step 2. Solve the system

$$\begin{aligned} A\alpha + B\beta &= b \\ B^T \alpha &= \gamma \quad \text{on } A_k \\ \beta &= 0 \quad \text{on } I_k. \end{aligned}$$

Step 3. Stop or set $k = k + 1$, $\alpha^k = \alpha$ and $\beta^k = \beta$, where α and β are the solutions of the system in *Step 2*.

5.2. Numerical Experiments. In this section, we present some numerical experiments to illustrate the theoretical results derived in this article. For this, we consider the computational domain to be the unit cube $\Omega = (0, 1)^3$ in \mathbb{R}^3 and the obstacle function to be $\chi \equiv 0$. Further the force function f is taken as

$$(5.2) \quad f(x, y, z) := \begin{cases} -4(2r^2 + 3(r^2 - r_0^2)) & \text{if } r > r_0, \\ -8r_0^2(1 - r^2 + r_0^2) & \text{if } r \leq r_0, \end{cases}$$

where $r = (x^2 + y^2 + z^2)^{1/2}$ and $r_0 = 7$. The nonhomogeneous Dirichlet boundary condition is taken in such a way that the solution u is given by $u(x, y, z) = (\max(r^2 - r_0^2, 0))^2$. The *Algorithm 5.1* is used in computations with $c = 1$ in the *Step 1* therein. In the experiment, we compute the order of convergence in the energy norm to test the performance of the result in Theorem 3.2. We begin with an initial mesh given in Figure 5.1 and generate an array of uniformly refined meshes by tetrahedrons by dividing each tetrahedron into 12 tetrahedrons. We compute the discrete solution on these meshes and then compute the corresponding errors using a quadrature formula that is exact for cubic polynomials. The results are depicted in the Table 5.1. The results match closely with the theoretical results. We have developed our in-house MATLAB code for this experiment. The discrete and the exact (interpolation) solutions are plotted in Figure 5.2 on the mesh with mesh $h = 0.433$ (around 1.03 Lakh tetrahedrons).

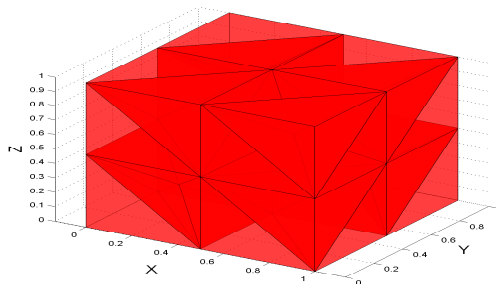


FIGURE 5.1. The initial mesh in computations

| h | $\ \nabla(u - u_h)\ _{L^2(\Omega)}$ | order |
|--------|-------------------------------------|--------|
| 0.3467 | 1.8500e-001 | — |
| 0.1733 | 5.6046e-002 | 1.3596 |
| 0.0867 | 1.9210e-002 | 1.4112 |
| 0.0433 | 7.1151e-003 | 1.3636 |

TABLE 5.1. Errors and order of convergence in H^1 norm

Numerical experiments to test the performance of a posteriori error estimates will be discussed in the future work.

6. CONCLUSIONS

We have developed a quadratic finite element method for the three dimensional elliptic obstacle problem. The finite element space is constructed by using the standard P_2 Lagrange finite element and a space of element-wise bubble functions. This enables us to prove optimal order (with respect to the regularity) error estimate in the energy norm. A posteriori error estimates are derived by constructing a suitable Lagrange multiplier. Further, a primal-dual active set method is proposed for the numerical implementation and a numerical experiment is presented to illustrate the theoretical result on *a priori* error estimate.

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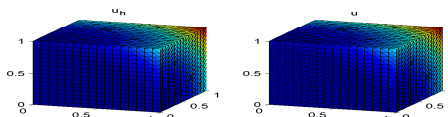


FIGURE 5.2. The comparison between the computed (left) and the exact (right) solution

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